Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 4230 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.14e-01

Confidence level: 5.24e-01

Nearest Neighbors from the Training Set

Image not found
C.I. Solvent Yellow 14
Measured: 3800
Predicted: 4350

Image not found
2-Aminoanthracene
Measured: 28200
Predicted: 24300

Image not found
3,3'-Dichlorobenzidine
Measured: 22400
Predicted: 1680

Image not found
Ethyl 1-naphthaleneacetate
Measured: 302
Predicted: 425

Image not found
2-Acetylaminofluorene
Measured: 1380
Predicted: 1860